

Supporting Information

A High-Affinity ^{64}Cu -Labeled Ligand for PET Imaging of Hepsin: Design, Synthesis, and Characterization

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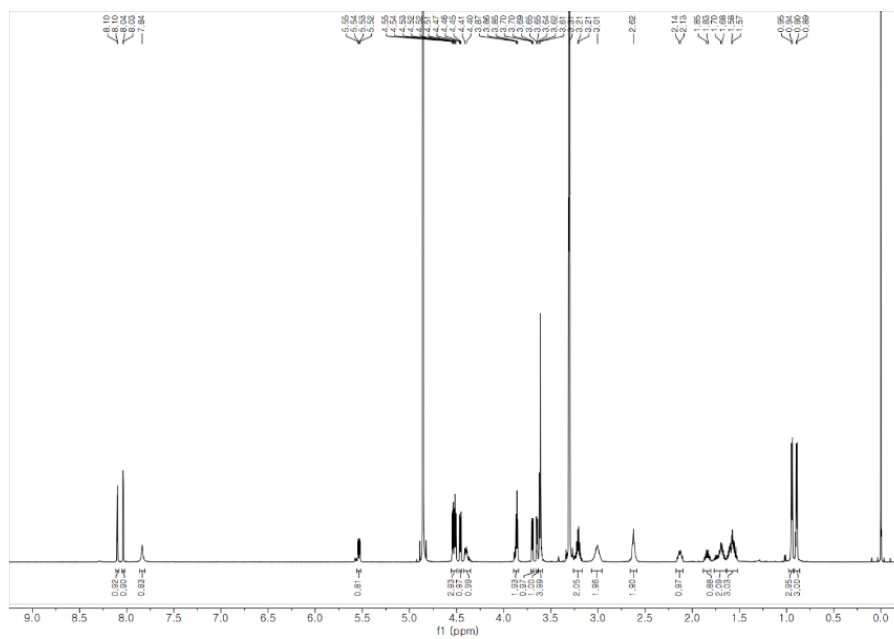
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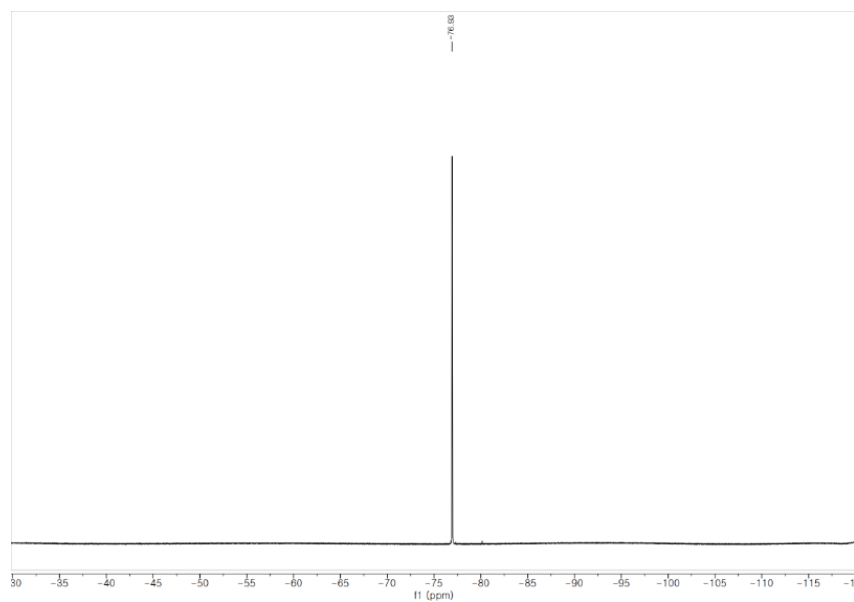
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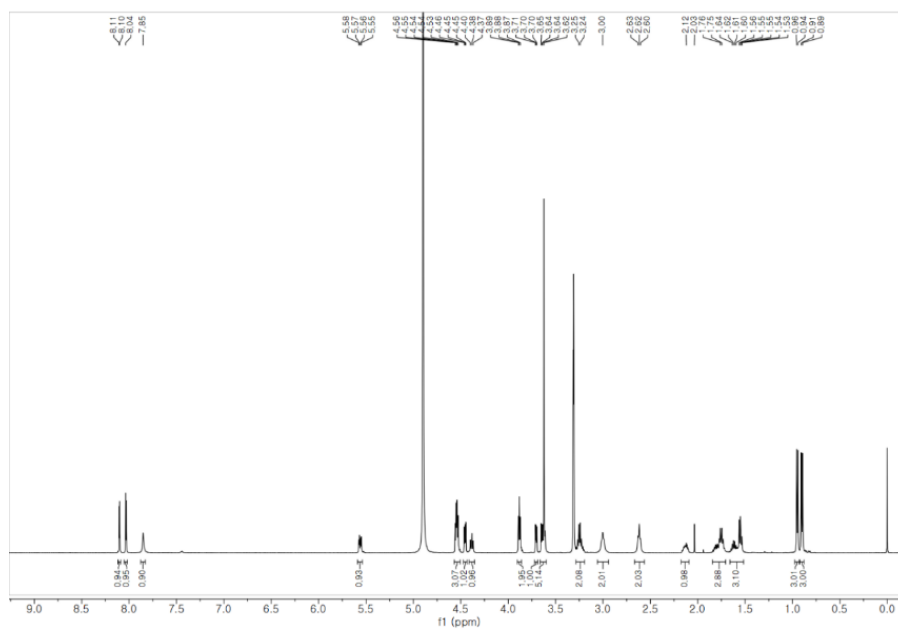
^1H and ^{19}F NMR spectra of 1A and 1B



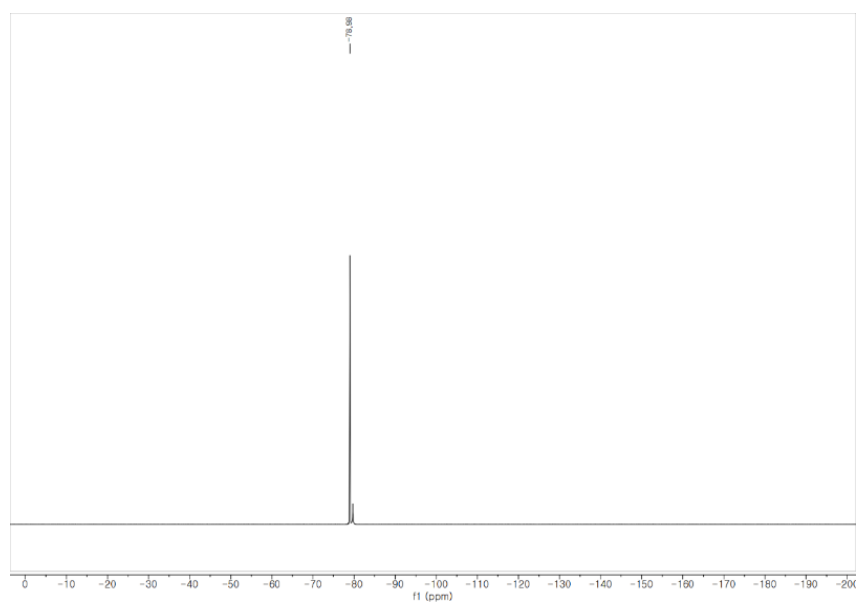
^1H NMR spectrum of ligand 1A



^{19}F NMR spectrum of ligand 1A

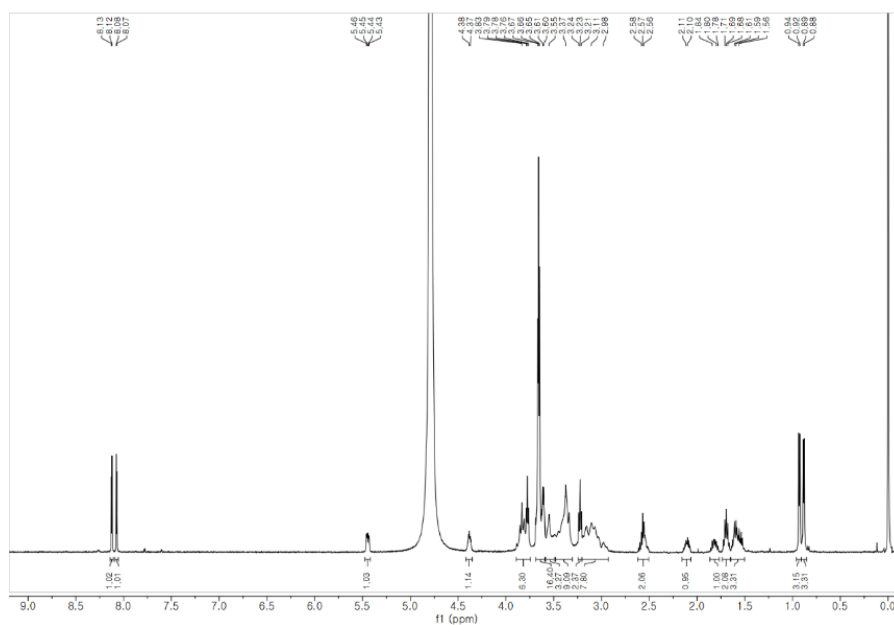


¹H NMR spectrum of ligand **1B**

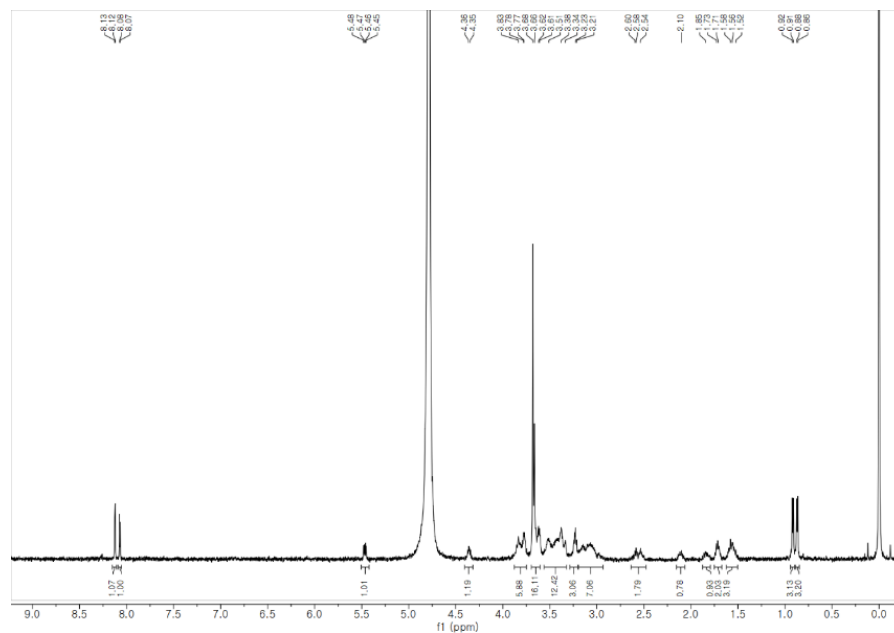


¹⁹F NMR spectrum of ligand **1B**

^1H NMR spectra of **11A** and **11B**

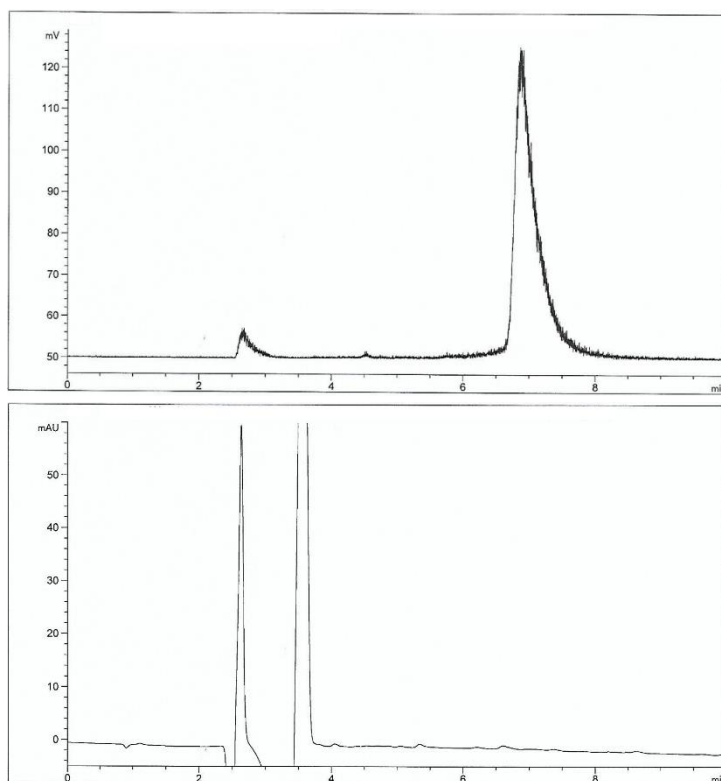


^1H NMR spectrum of **11A**



^1H NMR spectrum of **11B**

HPLC chromatograms of [⁶⁴Cu]3B



HPLC column: YMC-Pack C18, 4.6 × 250 mm, 5 μm

HPLC solvents: 75:25 water (0.1% TFA) — acetonitrile (0.1% TFA); flow rate: 1 mL/min

Detection: Radioactivity detector (top) and UV detector (230 nm) (bottom)

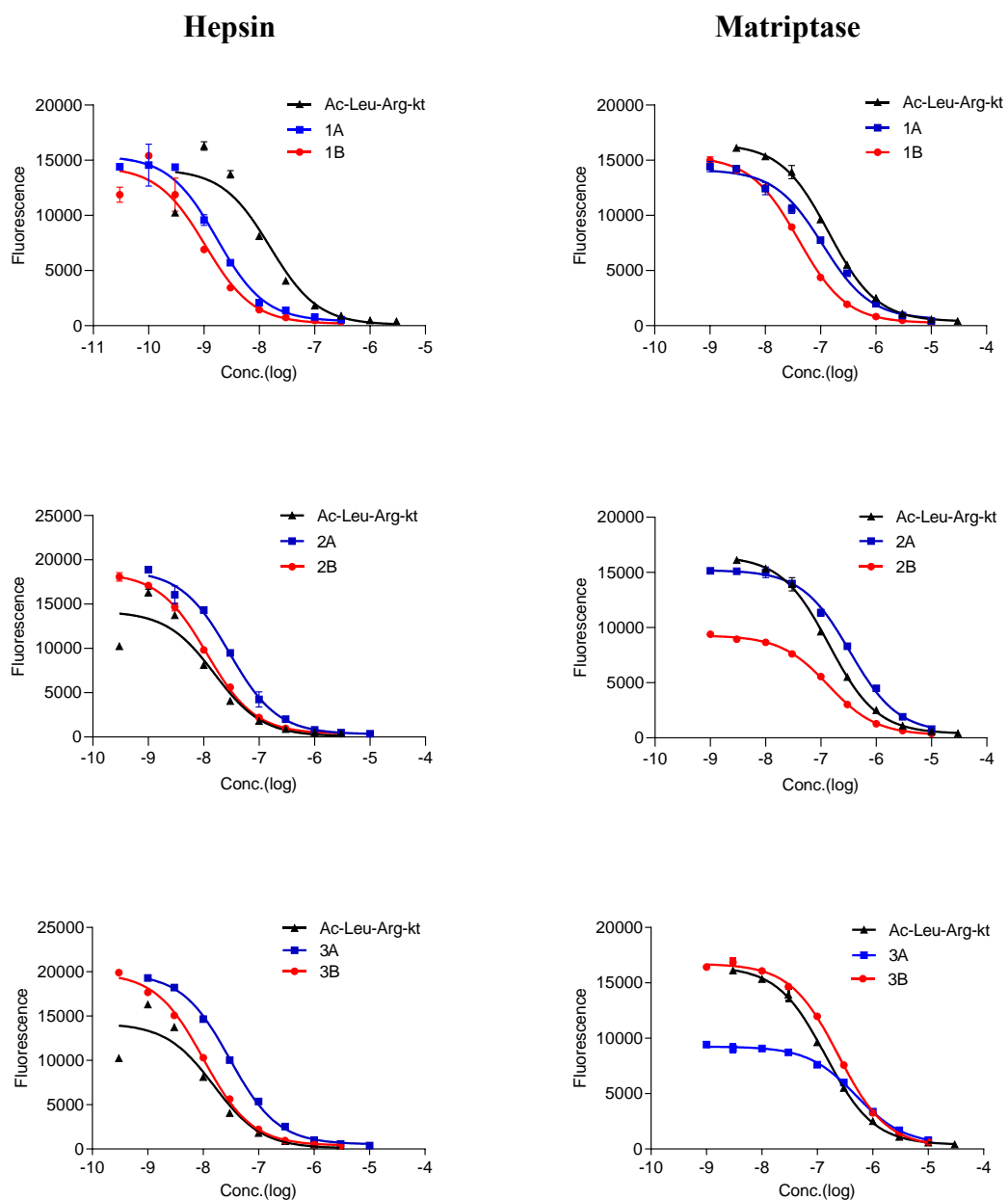
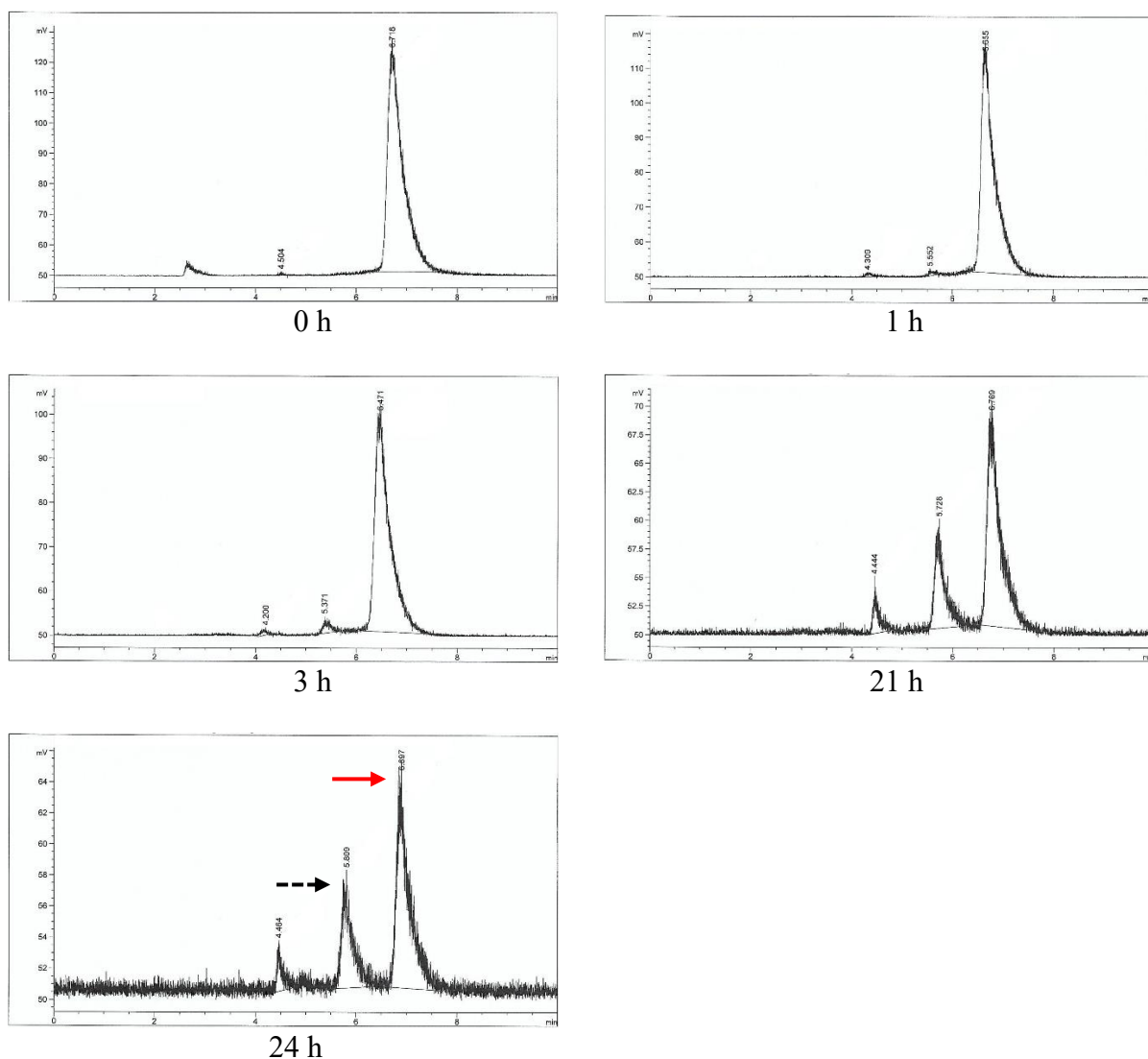


Figure S1. IC₅₀ curves of all six ligands for hepsin (left) and matriptase (right).



$[^{64}\text{Cu}]\mathbf{3B}$ (red solid arrow); $[^{64}\text{Cu}]\mathbf{3A}$ (black dotted arrow)

HPLC column: YMC-Pack C18, 4.6×250 mm, $5 \mu\text{m}$

HPLC solvents: 75:25 water (0.1% TFA) — acetonitrile (0.1% TFA)

Flow rate: 1 mL/min

Detection: Radioactivity detector

Figure S2. In vitro serum stability of $[^{64}\text{Cu}]\mathbf{3B}$.